

CHEMICAL PHYSICS LETTERS

Chemical Physics Letters 342 (2001) 674-684

www.elsevier.com/locate/cplett

Author Index to Volume 342

Abergel, D., see de Sousa, P.L.	342 (2001) 45
Adamowicz, L., see Smets, J.	342 (2001) 342
Aguirre, F., see Husband, J.	342 (2001) 75
Alonso, J.L., see Sanz, M.E.	342 (2001) 31
Alvarez, L., T. Guillard, J.L. Sauvajol, G. Flamant and D. Laplaze, Growth	
mechanisms and diameter evolution of single wall carbon nanotubes	342 (2001) 7
Amor, N.B., see Bossert, J.	342 (2001) 617
Andersen, J.N., see Over, H.	342 (2001) 467
Andrés, J., M. Canle L., M.V. García, L.F. Rodríguez Vázquez and J.A.	
Santaballa, A B3LYP/6-31G** study on the chlorination of ammonia by hypo-	
chlorous acid	342 (2001) 405
Ashok, V., see Rosa, A.	342 (2001) 536
Asirvatham, P.S., see Subramanian, V.	342 (2001) 603
Ausman, K.D., see O'Connell, M.J.	342 (2001) 265
Ba, Xw., see Wang, Hj.	342 (2001) 347
Balakrishnan, R., see Subramanian, V.	342 (2001) 603
Ball, S.M., I.M. Povey, E.G. Norton and R.L. Jones, Broadband cavity ringdown	
spectroscopy of the NO ₃ radical	342 (2001) 113
Baluja, S., see Matsuo, T.	342 (2001) 22
Barbara, P.F., see Hee Son, D.	342 (2001) 571
Bardeen, C.J., see Lim, SH.	342 (2001) 555
Barszczewska, W., see Rosa, A.	342 (2001) 536
Bartels, D.M., see Lossack, A.M.	342 (2001) 524
Bauschlicher, C.W. and H. Partridge, On interpreting the photoelectron spectra of	
MgO^-	342 (2001) 441
Beutl, M., J. Lesnik, K.D. Rendulic, R. Hirschl, A. Eichler, G. Kresse and J. Hafner,	
There is a true precursor for hydrogen adsorption after all: the system H ₂ /	
Pd(111)+subsurface V	342 (2001) 473
Bhavana, P., see Bhyrappa, P.	342 (2001) 39
Bhyrappa, P. and P. Bhavana, Unusual solvent dependent optical absorption spectral	
properties of free-base perhaloporphyrins	342 (2001) 39
Bian, G., see Sun, Z.	342 (2001) 323
Bielschowsky, C.E., see Borges, I.	342 (2001) 411
Billing, G.D., see Coletti, C.	342 (2001) 65
Bittl, R., see Fursman, C.E.	342 (2001) 162
Bjorklund, T.G., see Lim, SH.	342 (2001) 555
Bohr, F., see Henon, E.	342 (2001) 659

Borges, I. and C.E. Bielschowsky, On the semiclassical dissociation yields of the doubly	
excited states of H ₂	342 (2001) 411
Bossert, J., N.B. Amor, A. Strich and C. Daniel, Electronic spectroscopy of	312 (2001) 411
HRe(CO) ₅ : a CASSCF/CASPT2 and TD-DFT study	342 (2001) 617
Boul, P., see O'Connell, M.J.	342 (2001) 265
Bowman, J.M., see Carter, S.	342 (2001) 636
Braams, B.J., see Carter, S.	342 (2001) 636
Bradforth, S.E., see Lenchenkov, V.	342 (2001) 277
Branson, K., see Smith, B.J.	342 (2001) 402
Brüning, F., see Rosa, A.	342 (2001) 536
Budnik, B.A., K.F. Haselmann and R.A. Zubarev, Electron detachment dissociation of	
peptide di-anions: an electron-hole recombination phenomenon	342 (2001) 299
Burgers, P.C., see Ruttink, P.J.A.	342 (2001) 447
Cai, W., B. Xia, X. Shao, Q. Guo, B. Maigret and Z. Pan, Molecular docking of	
α-cyclodextrin inclusion complexes by genetic algorithm and empirical binding	a
free energy function	342 (2001) 387
Campos-Martínez, J., see di Domenico, D.	342 (2001) 177
Canle L., M., see Andrés, J.	342 (2001) 405
Cao, A., H. Zhu, X. Zhang, X. Li, D. Ruan, C. Xu, B. Wei, J. Liang and D. Wu,	(2001)
Hydrogen storage of dense-aligned carbon nanotubes	342 (2001) 510
Caporossi, G., see Fowler, P.W.	342 (2001) 105
Carter, S., J.M. Bowman and B.J. Braams, On using low-order Hermite interpolation in 'direct dynamics' calculations of vibrational energies using the code 'MULTI-	DS 17 M - M 10 1
MODE'	342 (2001) 636
Celebre, G., The orientational ordering of a biaxial particle in a uniaxial environment	342 (2001) 030
by Monte Carlo sampling: a new approach to the problem	342 (2001) 375
Clark, R.J.H., see Zhu, Y.Q.	342 (2001) 15
Coletti, C. and G.D. Billing, Quantum dressed classical mechanics: application to	342 (2001) 13
chemical reactions	342 (2001) 65
Corni, S. and J. Tomasi, Theoretical evaluation of Raman spectra and enhancement	5.2 (2001) 05
factors for a molecule adsorbed on a complex-shaped metal particle	342 (2001) 135
autors for a morecule ausoroea on a complex shaped metal particle	0.12 (2001) 100
Dai, J., see Sun, Z.	342 (2001) 323
Dai, L., see Hassanien, A.	342 (2001) 479
Dang, H.Y., see Tang, C.C.	342 (2001) 492
Daniel, C., see Bossert, J.	342 (2001) 617
de la Chapelle, M.L., see Tang, C.C.	342 (2001) 492
de Sousa, P.L., D. Abergel and JY. Lallemand, Experimental time saving in NMR	
measurement of time dependent diffusion coefficients	342 (2001) 45
Dellero, T., see Smiljanic, O.	342 (2001) 503
Désilets, S., see Smiljanic, O.	342 (2001) 503
di Domenico, D., M.I. Hernández and J. Campos-Martínez, A time-dependent wave	THE RESIDENCE OF THE PARTY OF T
packet approach for reaction and dissociation in $H_2 + H_2$	342 (2001) 177
Ding, L., see Sun, Z.	342 (2001) 323
Dodelet, J.P., see Smiljanic, O.	342 (2001) 503
Dopfer, O., see Solcà, N.	342 (2001) 191
Drickamer, H.G., see Zhu, A.	342 (2001) 337

Edén, M., see Zhao, X.	342 (2001) 353
Eichler, A., see Beutl, M.	342 (2001) 473
Endo, S., see Yamashita, H.	342 (2001) 382
Ericson, L.M., see O'Connell, M.J.	342 (2001) 265
Erman, P., Comment on measurements of the collisional deactivation rate of the	0.12 (2001) 200
$N_2C^3\Pi_{\mu}$ state	342 (2001) 515
and the said the	312 (2001) 313
Fakis, M., G. Tsigaridas, I. Polyzos, V. Giannetas, P. Persephonis, I. Spiliopoulos and	
J. Mikroyannidis, Intensity dependent nonlinear absorption of pyrylium chromo-	01000000
• phores • •	342 (2001) 155
Fan, S.S., see Tang, C.C.	342 (2001) 492
Fang, WH., see Zheng, X.	342 (2001) 425
Figari, G. and V. Magnasco, A simple polynomial approach to the exact perturbative	
evaluation of low-frequency dynamic polarizabilities for a ground-state hydrogen	0.000
atom	342 (2001) 99
Firth, S., see Zhu, Y.Q.	342 (2001) 15
Flamant, G., see Alvarez, L.	342 (2001) 7
Fowler, P.W., P. Hansen, G. Caporossi and A. Soncini, Polyenes with maximum)
HOMO-LUMO gap	342 (2001) 105
Fowler, P.W., R.W.A. Havenith and E. Steiner, Unconventional ring currents in an	342 (2001) 103
o 'all-metal aromatic', Al_4^{2-}	342 (2001) 85
Fowler, P.W., see László, I.	342 (2001) 369
Francisco, J.S., see Sandhyarani, N.	342 (2001) 272
Fuß, W., W.E. Schmid and S.A. Trushin, Ultrafast electronic relaxation of s-trans-	342 (2001) 272
butadiene	342 (2001) 91
Fursman, C.E., R. Bittl, S.G. Zech and P.J. Hore, 95 GHz ESEEM of radical pairs: a	342 (2001) 31
source of radical separations and relative orientations	342 (2001) 162
Furuhashi, O., T. Kinugawa, S. Masuda, C. Yamada and S. Ohtani, Double	342 (2001) 102
charge transfer spectroscopy of acetylene dication $C_2H_2^{2+}$ at vibrational	
resolution	342 (2001) 625
	342 (2001) 023
Galli, G., see Schwegler, E.	342 (2001) 434
Gao, H., see Li, J.	342 (2001) 529
Gao, M., see Hassanien, A.	342 (2001) 479
García, M.V., see Andrés, J.	342 (2001) 405
Garroway, A.N., see Sauer, K.L.	342 (2001) 362
Gauss, J., see Larsen, H.	342 (2001) 200
Giannetas, V., see Fakis, M.	342 (2001) 155
Goodings I M see Guo I	342 (2001) 169
Graovac A see László I	342 (2001) 369
Guillard, T., see Alvarez, L.	342 (2001) 7
Guo, J. and J.M. Goodings, A density-functional study of the reaction of neutral	342 (2001)
scandium with water	342 (2001) 169
Guo, Q., see Cai, W.	342 (2001) 387
Gygi, F., see Schwegler, E.	342 (2001) 434
-75, · · , · · · · · · · · · · · · · · · ·	342 (2001) 434
Hafner, J., see Beutl, M.	342 (2001) 473
Hansen, P., see Fowler, P.W.	342 (2001) 473
	342 (2001) 103

Harada, H., S. Shimizu, T. Yatsuhashi, S. Sakabe, Y. Izawa and N. Nakashima, A key factor in parent and fragment ion formation on irradiation with an intense	
femtosecond laser pulse	242 (2001) 562
	342 (2001) 563
Haroz, E., see O'Connell, M.J.	342 (2001) 265
Harrison, N.M., see Muscat, J.	342 (2001) 397
Haselmann, K.F., see Budnik, B.A.	342 (2001) 299
Hassanien, A., M. Gao, M. Tokumoto and L. Dai, Scanning tunneling microscopy of	
aligned coaxial nanowires of polyaniline passivated carbon nanotubes	342 (2001) 479
Havenith, R.W.A., see Fowler, P.W.	342 (2001) 85
Hazra, P. and N. Sarkar, Intramolecular charge transfer processes and solvation	
dynamics of coumarin 490 in reverse micelles	342 (2001) 303
Hee Son, D., P. Kambhampati, T.W. Kee and P.F. Barbara, One-photon UV	
detrapping of the hydrated electron	342 (2001) 571
Henon, E. and F. Bohr, Theoretical study of the H-abstraction reaction of the CH ₃ O	The three of a
radical with formaldehyde	342 (2001) 659
Hernández, M.I., see di Domenico, D.	342 (2001) 177
Hino, K., see Yamamoto, N.	342 (2001) 417
Hirschl, R., see Beutl, M.	342 (2001) 473
Hore, P.J., see Fursman, C.E.	342 (2001) 162
Horváth, D., see Jakab, É.	342 (2001) 317
Hsu, W.K., see Zhu, Y.Q.	342 (2001) 15
Huffman, C., see O'Connell, M.J.	342 (2001) 265
	342 (2001) 203
Husband, J., F. Aguirre, C.J. Thompson and R.B. Metz, Photodissociation spectra of transition metal sulfides: spin-orbit structure in charge transfer bands of FeS ⁺ and	242 (2001) 75
NiS ⁺	342 (2001) 75
Illenberger, E., see Rosa, A.	342 (2001) 536
Itoh, T., Fluorescence spectra and the 2 ¹ A _g level of 1,4-diphenylbutadiene in	
perfluorohexane and perfluoropentane	342 (2001) 550
Izawa, Y., see Harada, H.	342 (2001) 563
11.77 - 111.	212 (2001) 505
Jakab, É., D. Horváth, Á. Tóth, J.H. Merkin and S.K. Scott, The effect of reversible	
binding of the autocatalyst on the lateral instability of reaction fronts	342 (2001) 317
Jalbout, A.F., see Smets, J.	342 (2001) 342
Jaszewski, A.R., HDF and QCI studies on the heterosubstituted iminoxy radicals:	342 (2001) 342
substituent effect on the isotropic hyperfine couplings with ¹³ C and ¹ H nuclei	342 (2001) 239
Jones, R.L., see Ball, S.M.	342 (2001) 239
	,
Jørgensen, P., see Larsen, H.	342 (2001) 200
Jungwirth, P., Chemical oscillations based on photoautocatalysis of ozone	342 (2001) 287
Kambhampati, P., see Hee Son, D.	342 (2001) 571
Kee, T.W., see Hee Son, D.	342 (2001) 571
Keske, J.C. and B.H. Pate, High-sensitivity infrared-microwave-microwave triple-	
resonance spectroscopy of isomerizing molecules	342 (2001) 51
Kidera, A., see Yamashita, H.	342 (2001) 382
Kim, H.L., see Oh, C.Y.	342 (2001) 27
Kim, M.S., see Sung, B.J.	342 (2001) 610
Kimura, J., see Ohno, K.	342 (2001) 207
	()

and the second s	
Kinugawa, T., see Furuhashi, O.	342 (2001) 625
Kiyoshima, T. and S. Sato, Correlation of lifetimes observed in two vibrational levels	
of the $H_2EF^1\Sigma_g^+$ state	342 (2001) 461
Kloepfer, J., see Lenchenkov, V.	342 (2001) 277
Knowles, P.J., see Manby, F.R.	342 (2001) 599
Koike, Y., see Matsuo, T.	342 (2001) 22
Komasa, J. and J. Rychlewski, 2 ¹ P state of Be from exponentially correlated Gaussian functions	342 (2001) 185
Koslowski, T. and P. Vöhringer, Is solvated I ₃ angular?	342 (2001) 141
Kresse, G., see Beutl, M.	342 (2001) 473
Krimm, S., see Lee, SH.	342 (2001) 643
Krishna, R., see Paschek, D.	342 (2001) 148
Krishnakumar, E., see Rosa, A.	342 (2001) 536
Kroto, H.W., see Zhu, Y.Q.	342 (2001) 336
Kumar, S.V.K., see Rosa, A.	342 (2001) 536
Kuper, C., see O'Connell, M.J.	342 (2001) 330 342 (2001) 265
Ruper, C., see O Connen, W.J.	342 (2001) 203
Lallemand, JY., see de Sousa, P.L.	342 (2001) 45
Laplaze, D., see Alvarez, L.	342 (2001) 7
Larsen, H., J. Olsen, P. Jørgensen and J. Gauss, Comparison of full-configuration interaction and coupled-cluster harmonic and fundamental frequencies for BH and	
HF	342 (2001) 200
László, I., A. Rassat, P.W. Fowler and A. Graovac, Topological coordinates for	(2001) 200
toroidal structures	342 (2001) 369
Lebrun, G., see Smiljanic, O.	342 (2001) 503
Lee Phillips, D., see Zheng, X.	342 (2001) 425
Lee, C.S., see Tang, Y.H.	342 (2001) 259
Lee, SH., K. Palmo and S. Krimm, A new method to calculate B-matrix elements for	212 (2001) 203
external rotations with application to the B-matrix internal coordinate molecular	
dynamics formalism	342 (2001) 643
Lee, S.T., see Tang, Y.H.	342 (2001) 259
Lenchenkov, V., J. Kloepfer, V. Vilchiz and S.E. Bradforth, Electron photodetachment	342 (2001) 23)
from $[Fe(CN)_6]^{4-}$: photoelectron relaxation and geminate recombination	342 (2001) 277
Lesnik, J., see Beutl, M.	342 (2001) 473
Levitt, M.H., see Zhao, X.	342 (2001) 353
Li, J., L. Wu and Y. Zhang, Theoretical study of adsorbed-decomposition of NO, CO	342 (2001) 333
and CH_2O on a $TiO_2(110)$ (1×1) defect surface	342 (2001) 249
Li, J., X. Shen and H. Gao, Exploring the locations of different groups of a cationic surface-active 3 <i>H</i> -indole probe molecule in AOT-based water-in-oil microemulsions	342 (2001) 529
Li, P., see Tang, C.C.	
	342 (2001) 492
Li, X., see Cao, A.	342 (2001) 510
Li, Y., see Lu, X.	342 (2001) 545
Li, ZS., see Wang, Hj.	342 (2001) 347
Liang, J., see Cao, A.	342 (2001) 510
Lim, SH., T.G. Bjorklund and C.J. Bardeen, Temperature-dependent exciton	
dynamics in poly(p-phenylene vinylene) measured by femtosecond transient spectroscopy	342 (2001) 555
spectroscopy	342 (2001) 555

Lin I see In V	242 (2001) 545
Liu, J., see Lu, X. Liu, Y.M., see Tang, C.C.	342 (2001) 545
López, J.C., see Sanz, M.E.	342 (2001) 492
Lossack, A.M., E. Roduner and D.M. Bartels, Kinetics of the reaction of H and D with	342 (2001) 31
methanediol and 1,2-ethanediol in aqueous solution	342 (2001) 524
Lu, QB., T.E. Madey, L. Parenteau, F. Weik and L. Sanche, Structural and	342 (2001) 324
temperature effects on Cl ⁻ yields in electron-induced dissociation of CF ₂ Cl ₂	
adsorbed on water ice	342 (2001) 1
Lu, X., H. Zhang, Y. Li, J. Liu and G. Yang, High pressure effects on the luminescent	342 (2001)
properties and crystal structure of magnesium 8-hydroxyquinoline complex	342 (2001) 545
Lundgren, E., see Over, H.	342 (2001) 467
Editagren, 2., see ever, 11.	342 (2001) 407
Madey, T.E., see Lu, QB.	342 (2001) 1
Magnasco, V., see Figari, G.	342 (2001) 99
Maigret, B., see Cai, W.	342 (2001) 387
Manby, F.R., R.P. Tuckett and P.J. Knowles, A theoretical study of the electronic	()
spectroscopy of the SiF ₃ radical	342 (2001) 599
Masuda, S., see Furuhashi, O.	342 (2001) 625
Matsuo, T., S. Baluja, Y. Koike, M. Ohama, T. Mochida and T. Sugawara,	, , , , ,
Spectroscopic and calorimetric studies of proton tunneling and deuteration-induced	
phase transition in crystalline iodo-hydroxyphenalenone and iodo-deuteroxyphe-	
nalenone	342 (2001) 22
McDowell, S.A.C., Are H-He-Cl and H-Ne-Cl metastable species? A computational	
study	342 (2001) 631
Merkin, J.H., see Jakab, É.	342 (2001) 317
Metz, R.B., see Husband, J.	342 (2001) 75
Michel-Beyerle, ME., see Voityuk, A.A.	342 (2001) 231
Mikroyannidis, J., see Fakis, M.	342 (2001) 155
Miller, J.B., see Sauer, K.L.	342 (2001) 362
Mio, M.J., see Zhu, A.	342 (2001) 337
Mochida, T., see Matsuo, T.	342 (2001) 22
Mogi, K., see Yamamoto, N.	342 (2001) 417
Mohanty, J., H. Pal, R.D. Saini and A.V. Sapre, Triplet state characteristics of 2,2'-	
and 4,4'-biphenyldiols studied by 248 nm nanosecond laser flash photolysis	342 (2001) 328
Molski, M., Dipole moment of $ArH^+X^1\Sigma^+$ from analysis of pure rotational and	
vibration-rotational spectra	342 (2001) 293
Moon, J.H., see Sung, B.J.	342 (2001) 610
Moore, J.S., see Zhu, A.	342 (2001) 337
Moscardó, F., see Sancho-García, J.C.	342 (2001) 452
Muscat, J., A. Wander and N.M. Harrison, On the prediction of band gaps from	
hybrid functional theory	342 (2001) 397
Nagashima II saa Okamata M	242 (2001) 579
Nagashima, H., see Okamoto, M.	342 (2001) 578 342 (2001) 58
Nakahara, H., see Ray, K.	342 (2001) 58 342 (2001) 563
Nakashima, N., see Harada, H.	342 (2001) 563 342 (2001) 536
Nandi, D., see Rosa, A.	342 (2001) 536 342 (2001) 113
Norton, E.G., see Ball, S.M.	342 (2001) 113

O'Connell, M.J., P. Boul, L.M. Ericson, C. Huffman, Y. Wang, E. Haroz, C. Kuper, J.	
Tour, K.D. Ausman and R.E. Smalley, Reversible water-solubilization of single-	
walled carbon nanotubes by polymer wrapping	342 (2001) 265
Oh, C.Y., S.K. Shin, H.L. Kim and C.R. Park, Photodissociation of allyl cyanide at	
193 nm	342 (2001) 27
Ohama, M., see Matsuo, T.	342 (2001) 22
Ohashi, K., see Yamamoto, N.	342 (2001) 417
Ohno, K., J. Kimura and Y. Yamakita, Strong Raman activities of low frequency	
vibrational modes in alkylbenzenes: conformation specific σ - π interactions between	
alkyl chain and benzene ring	342 (2001) 207
Ohtani, S., see Furuhashi, O.	342 (2001) 625
Okamoto, M., K. Yamada, H. Nagashima and F. Tanaka, Fluorescence quenching of	
9,10-dicyanoanthracene by oxygen in liquid and supercritical carbon dioxide	342 (2001) 578
Olsen, J., see Larsen, H.	342 (2001) 200
Orzechowski, K., see Szala, A.	342 (2001) 519
Over, H., A.P. Seitsonen, E. Lundgren, M. Wiklund and J.N. Andersen, Spectroscopic	
characterization of catalytically active surface sites of a metallic oxide	342 (2001) 467
	()
Pal, H., see Mohanty, J.	342 (2001) 328
Pal, S., Erratum to: "Partial double- and single-differential cross-sections for CO2 by	
electron collision" [Chem. Phys. Lett. 308 (1999) 428]	342 (2001) 673
Palmo, K., see Lee, SH.	342 (2001) 643
Pan, Z., see Cai, W.	342 (2001) 387
Parenteau, L., see Lu, QB.	342 (2001) 1
Park, C.R., see Oh, C.Y.	342 (2001) 27
Pérez-Jiménez, A.J., see Sancho-García, J.C.	342 (2001) 452
Pérez-Jordá, J.M., see Sancho-García, J.C.	342 (2001) 452
Partridge, H., see Bauschlicher, C.W.	342 (2001) 441
Pascal, R.A., see Soos, Z.G.	342 (2001) 652
Paschek, D. and R. Krishna, Monte Carlo simulations of sorption and diffusion of	()
isobutane in silicalite	342 (2001) 148
Pate, B.H., see Keske, J.C.	342 (2001) 51
Persephonis, P., see Fakis, M.	342 (2001) 155
Pinčák, R., see Pudlak, M.	342 (2001) 587
Polyzos, I., see Fakis, M.	342 (2001) 155
Povey, I.M., see Ball, S.M.	342 (2001) 113
Pradeep, T., see Sandhyarani, N.	342 (2001) 272
Pudlak, M. and R. Pinčák, The role of accessory bacteriochlorophylls in the primary	()
charge transfer in the photosynthetic reaction centers	342 (2001) 587
Qi, F., see Zhong, S.	342 (2001) 583
Rakitzis, T.P., Direct measurement of photofragment alignment from unnormalized	
Abel-invertible images	342 (2001) 121
Ramamoorthy, A., see Shekar, S.C.	342 (2001) 127
Ramamoorthy, A., see Wei, Y.	342 (2001) 312
Ramasami, T., see Subramanian, V.	342 (2001) 603
Rassat, A., see László, I.	342 (2001) 369
	2.2 (2001) 505

Ray, K., H. Nakahara, A. Sakamoto and M. Tasumi, Excitation energy transfer	
from symmetric cyanine dyes to unsymmetric merocyanine aggregated in	
functionalized Langmuir-Blodgett films by time-resolved fluorescence spectro-	
scopy	342 (2001) 58
Rendulic, K.D., see Beutl, M.	342 (2001) 473
Rode, M.F. and J. Sadlej, The (H ₂ O) ₂ CO ternary complex: cyclic or linear?	342 (2001) 220
Rodríguez Vázquez, L.F., see Andrés, J.	342 (2001) 405
Roduner, E., see Lossack, A.M.	342 (2001) 524
Rosa, A., W. Barszczewska, D. Nandi, V. Ashok, S.V.K. Kumar, E. Krishnakumar, F.	
Brüning and E. Illenberger, Unusual temperature dependence in dissociative	
electron attachment to 1,4-chlorobromobenzene	342 (2001) 536
Rösch, N., see Voityuk, A.A.	342 (2001) 231
Ruan, D., see Cao, A.	342 (2001) 510
Ruttink, P.J.A., P.C. Burgers, M.A. Trikoupis and J.K. Terlouw, The heat of	342 (2001) 310
formation of sulfine, CH ₂ =S=O, revisited: a CBS-QB3 study	342 (2001) 447
Rychlewski, J., see Komasa, J.	342 (2001) 185
Rychiewski, J., see Romasa, J.	342 (2001) 183
Cadlei I and Dada M.E.	242 (2001) 220
Sadlej, J., see Rode, M.F.	342 (2001) 220
Saini, R.D., see Mohanty, J.	342 (2001) 328
Sakabe, S., see Harada, H.	342 (2001) 563
Sakai, Y., see Yamamoto, N.	342 (2001) 417
Sakamoto, A., see Ray, K.	342 (2001) 58
Salafsky, J.S., 'SHG-labels' for detection of molecules by second harmonic generation	342 (2001) 485
Sanche, L., see Lu, QB.	342 (2001) 1
Sancho-García, J.C., A.J. Pérez-Jiménez, J.M. Pérez-Jordá and F. Moscardó, High-	
level ab initio calculations of the torsional potential of glyoxal	342 (2001) 452
Sandhyarani, N., T. Pradeep and J.S. Francisco, Radical-induced core destruction of	
monolayer-protected metal clusters	342 (2001) 272
Santaballa, J.A., see Andrés, J.	342 (2001) 405
Sanz, M.E., V.M. Sanz, J.C. López and J.L. Alonso, Oxetane-hydrogen fluoride	
complex: a rotational study	342 (2001) 31
Sanz, V.M., see Sanz, M.E.	342 (2001) 31
Sapre, A.V., see Mohanty, J.	342 (2001) 328
Sarkar, N., see Hazra, P.	342 (2001) 303
Sato, S., see Kiyoshima, T.	342 (2001) 461
Sauer, K.L., B.H. Suits, A.N. Garroway and J.B. Miller, Three-frequency nuclear	
quadrupole resonance of spin-1 nuclei	342 (2001) 362
Sauvajol, J.L., see Alvarez, L.	342 (2001) 7
Schmid, W.E., see Fuß, W.	342 (2001) 91
Schüürmann, G., see Smith, B.J.	342 (2001) 402
Schwegler, E., G. Galli and F. Gygi, Conformational dynamics of the dimethyl	312 (2001) 102
phosphate anion in solution	342 (2001) 434
Scott, S.K., see Jakab, É.	342 (2001) 317
	342 (2001) 467
Seitsonen, A.P., see Over, H.	342 (2001) 407
Sekiya, II., see Tamamoto, N.	
Serventi, A., see Smiljanic, O.	342 (2001) 503
Sham, T.K., see Tang, Y.H.	342 (2001) 259
Shao, X., see Cai, W.	342 (2001) 387

Shekar, S.C. and A. Ramamoorthy, The unitary evolution operator for cross- polarization schemes in NMR	342 (2001) 12
Shen, X., see Li, J.	342 (2001) 52
Shimizu, S., see Harada, H.	342 (2001) 56
Shin, S.K., see Oh, C.Y.	342 (2001) 2
	342 (2001) 2
Slabanja, M. and Gö. Wahnström, Quantum path-integral simulation of poly(propy-	242 (2001) 50
lene oxide)	342 (2001) 59
Smalley, R.E., see O'Connell, M.J.	342 (2001) 26
Smets, J., A.F. Jalbout and L. Adamowicz, Anions of the hydrogen-bonded guanine-	
cytosine dimer – theoretical study	342 (2001) 34
Smiljanic, O., T. Dellero, A. Serventi, G. Lebrun, B.L. Stansfield, J.P. Dodelet, M.	
Trudeau and S. Désilets, Growth of carbon nanotubes on Ohmically heated carbon	
paper	342 (2001) 50
Smith, B.J., K. Branson and G. Schüürmann, Gaussian-theory predictions of proton	
transfer to water of phenol and 3-chlorophenol: resolution of an apparent difficulty	342 (2001) 40
Solcà, N. and O. Dopfer, Protonation of aromatic molecules: competition between ring	
and oxygen protonation of phenol (Ph) revealed by IR spectra of PhH ⁺ -Ar _n	342 (2001) 19
Soncini, A., see Fowler, P.W.	342 (2001) 10
Song, Y., see Suo, Z.	342 (2001) 49
Soos, Z.G., E.V. Tsiper and R.A. Pascal, Charge redistribution and electronic	(====) 12
polarization in organic molecular crystals	342 (2001) 65
Spiliopoulos, I., see Fakis, M.	342 (2001) 15
Stansfield, B.L., see Smiljanic, O.	342 (2001) 50
Steiner, E., see Fowler, P.W.	342 (2001) 8
Strich, A., see Bossert, J.	342 (2001) 61
Subramanian, V., P.S. Asirvatham, R. Balakrishnan and T. Ramasami, Molecular	342 (2001) 01
	342 (2001) 60
mechanics studies on polypropylene and polymethylmethacrylate polymers	,
Sugawara, T., see Matsuo, T.	342 (2001) 2
Suits, B.H., see Sauer, K.L.	342 (2001) 36
Sun, Z., M. Tong, H. Zeng, L. Ding, Z. Wang, Z. Xu, J. Dai and G. Bian, Optical	
limiting response in a unsymmetrical dithiolene metal complex	242 (2224) 22
$(Me_4N)_2[Zn(dmit)(Sph)_2]$	342 (2001) 32
Sung, B.J., J.H. Moon and M.S. Kim, Checking the influence of numerically induced	
chaos in the computational study of intramolecular dynamics using trajectory	
equivalence	342 (2001) 61
Suo, Z., Y. Song, S. Yao, Y. Wang and Z. Xu, Optical limiting performance of	
dicyanodihydrofullerene	342 (2001) 49
Szala, A. and K. Orzechowski, Influence of strong electric field on dielectric	
permittivity of polycrystalline ice at MHz frequencies	342 (2001) 51
Tamm, T., see Uudsemaa, M.	342 (2001) 66
Canaka, F., see Okamoto, M.	342 (2001) 57
Tang, C.C., M.L. de la Chapelle, P. Li, Y.M. Liu, H.Y. Dang and S.S. Fan, Catalytic	2.2 (2001) 37
growth of nanotube and nanobamboo structures of boron nitride	342 (2001) 49
	342 (2001) 49
Tang, Y.H., Y.F. Zheng, C.S. Lee, N. Wang, S.T. Lee and T.K. Sham, Carbon	242 (2001) 25
monoxide-assisted growth of carbon nanotubes	342 (2001) 259
asumi, M., see Ray, K.	342 (2001) 5
Ferlouw, J.K., see Ruttink, P.J.A.	342 (2001) 44

Terrones, M., see Zhu, Y.Q.	342 (2001) 15
Thompson, C.J., see Husband, J.	342 (2001) 75
Tokumoto, M., see Hassanien, A.	342 (2001) 479
Tomasi, J., see Corni, S.	342 (2001) 135
Tong, M., see Sun, Z.	342 (2001) 323
Tóth, Á., see Jakab, É.	342 (2001) 317
Tour, J., see O'Connell, M.J.	342 (2001) 265
Trikoupis, M.A., see Ruttink, P.J.A.	342 (2001) 447
Trudeau, M., see Smiljanic, O.	342 (2001) 503
Trushin, S.A., see Fuß, W.	342 (2001) 91
Tsigaridas, G., see Fakis, M.	342 (2001) 155
Tsiper, E.V., see Soos, Z.G.	342 (2001) 652
Tuckett, R.P., see Manby, F.R.	342 (2001) 599
Uudsemaa, M. and T. Tamm, Calculations of hydrated titanium ion complexes:	
structure and influence of the first two coordination spheres	342 (2001) 667
Vilchiz, V., see Lenchenkov, V.	342 (2001) 277
Vöhringer, P., see Koslowski, T.	342 (2001) 141
Voityuk, A.A., ME. Michel-Beyerle and N. Rösch, Energetics of excess electron	
transfer in DNA	342 (2001) 231
Wahnström, Gö., see Slabanja, M.	342 (2001) 593
Wako, H., see Yamashita, H.	342 (2001) 382
Walton, D.R.M., see Zhu, Y.Q.	342 (2001) 15
Wander, A., see Muscat, J.	342 (2001) 397
Wang, Hj., Xw. Ba, M. Zhao and ZS. Li, The scaling study for the hydrogen	3.97 O.7 m/S
bonding networks	342 (2001) 347
Wang, N., see Tang, Y.H.	342 (2001) 259
Wang, Y., see O'Connell, M.J.	342 (2001) 265
Wang, Y., see Suo, Z.	342 (2001) 497
Wang, Z., see Sun, Z.	342 (2001) 323
Wei, B., see Cao, A.	342 (2001) 510
Wei, Y. and A. Ramamoorthy, 2D ¹⁵ N- ¹⁵ N isotropic chemical shift correlation	
established by ¹ H- ¹ H dipolar coherence transfer in biological solids	342 (2001) 312
Weik, F., see Lu, QB.	342 (2001) 1
Wiklund, M., see Over, H.	342 (2001) 467
Wu, D., see Cao, A.	342 (2001) 510
Wu, L., see Li, J.	342 (2001) 249
Xia, B., see Cai, W.	342 (2001) 387
Xin, H., see Zhong, S.	342 (2001) 583
Xu, C., see Cao, A.	342 (2001) 510
Xu, Z., see Sun, Z.	342 (2001) 323
Xu, Z., see Suo, Z.	342 (2001) 497
Yamada, C., see Furuhashi, O.	342 (2001) 625
Yamada, K., see Okamoto, M.	342 (2001) 578

Yamakita, Y., see Ohno, K.	342 (2001) 207
Yamamoto, N., K. Hino, K. Mogi, K. Ohashi, Y. Sakai and H. Sekiya, Hole-burning	
spectroscopy and ab initio calculations for the aniline dimer	342 (2001) 417
Yamashita, H., S. Endo, H. Wako and A. Kidera, Sampling efficiency of molecular	
dynamics and Monte Carlo method in protein simulation	342 (2001) 382
Yang, G., see Lu, X.	342 (2001) 545
Yao, S., see Suo, Z.	342 (2001) 497
Yatsuhashi, T., see Harada, H.	342 (2001) 563
Zech, S.G., see Fursman, C.E.	342 (2001) 162
Zeng, H., see Sun, Z.	342 (2001) 323
Zhang, H., see Lu, X.	342 (2001) 545
Zhang, X., see Cao, A.	342 (2001) 510
Zhang, Y., see Li, J.	342 (2001) 249
Zhao, M., see Wang, Hj.	342 (2001) 347
Zhao, X., M. Edén and M.H. Levitt, Recoupling of heteronuclear dipolar interactions	
in solid-state NMR using symmetry-based pulse sequences	342 (2001) 353
Zheng, X., WH. Fang and D. Lee Phillips, Resonance Raman and ab initio	
investigation of I ₂ -olefin complexes	342 (2001) 425
Zheng, Y.F., see Tang, Y.H.	342 (2001) 259
Zhong, S., F. Qi and H. Xin, Internal stochastic resonance in a model system for	
intracellular calcium oscillations	342 (2001) 583
Zhu, A., M.J. Mio, J.S. Moore and H.G. Drickamer, A quantitative study of the	
volume changes resulting from pressure-induced unfolding of m-phenylene	
ethynylene foldamers in solid PMMA and PtBMA	342 (2001) 337
Zhu, H., see Cao, A.	342 (2001) 510
Zhu, Y.Q., W.K. Hsu, S. Firth, M. Terrones, R.J.H. Clark, H.W. Kroto and D.R.M.	
Walton, Nb-doped WS ₂ nanotubes	342 (2001) 15
Zubarev, R.A., see Budnik, B.A.	342 (2001) 299

